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Evaluation of Agricultural Production Systems Simulator as yield predictor of *Panicum virgatum* and *Miscanthus* x *giganteus* in several US environments

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Abstract

Simulation models for perennial energy crops such as switchgrass (*Panicum virgatum* L.) and *Miscanthus* (*Miscanthus* x *giganteus*) can be useful tools to design management strategies for biomass productivity improvement in US environments. The Agricultural Production Systems Simulator (APSIM) is a biophysical model with the potential to simulate the growth of perennial crops. APSIM crop modules do not exist for switchgrass and *Miscanthus*, however, re-parameterization of existing APSIM modules could be used to simulate the growth of these perennials. Our aim was to evaluate the ability of APSIM to predict the dry matter (DM) yield of switchgrass and *Miscanthus* at several US locations. The *Lucerne* (for switchgrass) and *Sugarcane* (for *Miscanthus*) APSIM modules were calibrated using data from four locations in Indiana. A sensitivity analysis informed the relative impact of changes in plant and soil parameters of APSIM *Lucerne* and APSIM *Sugarcane* modules. An independent dataset of switchgrass and *Miscanthus* DM yields from several US environments was used to validate these re-parameterized APSIM modules. The re-parameterized modules simulated DM yields of switchgrass [0.95 for CCC (concordance correlation coefficient) and 0 for SB (bias of the simulation from the measurement)] and *Miscanthus* (0.65 and 0% for CCC and SB, respectively) accurately at most locations with the exception of switchgrass at southern US sites (0.01 for CCC and 2% for SB). Therefore, the APSIM model is a promising tool for simulating DM yields for switchgrass and *Miscanthus* while accounting for environmental variability. Given our study was strictly based on APSIM calibrations at Indiana locations, additional research using more extensive calibration data may enhance APSIM robustness.

Keywords: Agricultural Production Systems Simulator, bioenergy, biomass, *Miscanthus*, model re-parameterization, switchgrass, United States

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Introduction

Many studies throughout US have reported the extraordinary potential for high biomass production of switchgrass (*Panicum virgatum* L.) (Vogel *et al*., 2002; Kiniry *et al*., 2012; Burks, 2013; Arundale *et al*., 2014; Trybula *et al*., 2014) and *Miscanthus* (*Miscanthus* x *giganteus*) (Heaton *et al*., 2004, 2008; Khanna *et al*., 2008; Jain *et al*., 2010; Kiniry *et al*., 2012; Mishra *et al*., 2013; Trybula *et al*., 2014), both perennial rhizomatous grasses with C4 photosynthesis. Stakeholders involved in developing biomass crops for bioenergy are therefore increasingly interested in estimating potential yields of both species over large geographical domains (Clifton-Brown *et al*., 2004). Direct measurements of dry matter (DM) yields of these species are scarce relative to corn (*Zea mays* L.), soybean (*Glycine max* [L.] Merr.) and other grain crop species, and this lack of data over large geographies and at a fine spatial resolution remains a limitation to informed decision making (Clifton-Brown *et al*., 2004).

Satisfactory predictions of switchgrass biomass production were achieved with models like ALMANAC in Texas, Arkansas and Louisiana (Kiniry *et al*., 2005) and SWAT in Indiana (Trybula *et al*., 2014). Stampfl *et al*. (2007) achieved satisfactory simulations of *Miscanthus* biomass production across diverse climate and soil

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conditions in Europe using the MISCANMOD model developed by Clifton-Brown *et al.* (2000, 2004). Likewise, European studies for renewable energy used a FORTRAN version of MISCANMOD (Hastings *et al.*, 2008) and showed satisfactory simulation of *Miscanthus* biomass production derived by model improvements in the drought stress function, temperature effect in radiation use efficiency (RUE) and the inclusion of photoperiodism effects (Hastings *et al.*, 2009). Parameterization of WINOWAC was also performed for *Miscanthus* (Miguez, 2007). Other examples of modelling growth/adaptation of these species include the use of the STELLA software (Pallipparambil *et al.*, 2015) to identify Ohio, Missouri, Arkansas and Illinois as suitable locations for *Miscanthus*, as well as to determine sensitive parameters for biomass production. In a recent study (Strullu *et al.*, 2015) the STICS crop-soil model accurately predicted *Miscanthus* biomass production and environmental impacts in various environments in France and the UK. Despite this important progress in the calibration, development, and modification of several simulation models, the ability to predict DM yield both of switchgrass and *Miscanthus* by a single model has not yet been achieved.

In this context, a model scaled for a large geographic region and demonstrating adequate performance to predict DM yield is needed. The Agricultural Production Systems Simulator (APSIM) (Keating *et al.*, 2003) is a biophysical model with potential to simulate growth of annual and perennial crops. The APSIM model has been developed in Australia to simulate, on a daily time step, the main biophysical processes of a generic plant in response to management and weather (Keating *et al.*, 2003; Holzworth *et al.*, 2014). However, without preexisting APSIM crop modules to simulate switchgrass and *Miscanthus*, the re-parameterization of other APSIM crop modules such as the APSIM *Lucerne* (Robertson *et al.*, 2002) and APSIM *Sugarcane* modules (Keating *et al.*, 1999) could act as alternatives to simulate growth of both crops. In order to allow the use of APSIM for this purpose, a supervised calibration with a detailed data base and an evaluation of its predictive ability over a broad range of soils and environments is required. Our objectives were to (i) calibrate APSIM *Lucerne* module for switchgrass and APSIM *Sugarcane* module for *Miscanthus* using experimental field data collected in several locations across Indiana and (ii) validate these re-parameterized APSIM modules with independent data from numerous US locations where the accuracy and biases were evaluated.

Materials and methods

The calibration of the APSIM *Lucerne* and APSIM *Sugarcane* modules was made using the following steps: (i) data on climate, soil, and management were collected for model inputs; (ii) soil parameterization by location; (iii) adaptation of original plant modules to model switchgrass and *Miscanthus* growth using actual data from literature or field experiments and (iv) sensitivity analysis to evaluate parameter influence on LAI and the DM yield. Outcomes of the sensitivity analysis by successive iterations directed the compilation of existing data and additional field measurements used to develop model parameters. The model was calibrated through graphical comparison and statistical analyses of observed and modelled leaf area index (LAI) and DM yield data from IN locations with the objective to increase the concordance correlation coefficient (CCC, Tedeschi, 2006) and decrease the bias of the simulation from the measurement (SB, Kobayashi & Us Salam, 2000). These data included not only detailed measurements of LAI and DM yields at the final harvest, but also during crop growth and development. Model validation was made by using graphical comparisons and statistical analyses of observed and modelled DM yield data from 35 locations across the US. Data for switchgrass were grouped by region (southern vs. northern locations) and ecotype (upland vs. lowland). A complete description of datasets used for calibration and validation are provided in the supplementary information (Tables S3 and S4).

Data for model simulations

The data used for model calibration were obtained from field trials across IN (Table 1). For switchgrass model calibration, data from the Water Quality Field Station at Purdue University Agronomy Center for Research and Education (ACRE) near West Lafayette (40°28′11.99″N; 87°0′36.00″W) and Throckmorton Purdue Agricultural Center (TPAC) five miles south of Lafayette in Tippecanoe County (40°17′59.99″N; 86°54′0.00″W) (Table 1). The *Miscanthus* calibration included two additional IN locations: Northeast Purdue Agricultural Center (NEPAC) in Whitley County between Fort Wayne and Columbia City (41°8′24.00″N; 85°29′23.99″W), and the Southeast Purdue Agricultural Center (SEPAC) six miles east of North Vernon in Jennings County (39° 1′48.00″N; 85°31′11.99″W) (Table 1). A complete description of datasets used for calibration and validation of the model is shown in the supplementary information (Tables S3 and S4 for switchgrass and *Miscanthus*, respectively). Subsequent model validation used data of DM yields gathered across the US, which were collected from published and unpublished studies from 34 dryland locations and one irrigated location (Davis, CA) in 16 states (Fig. 1; Table 1).

Climate data sources

Daily meteorological data for each location were derived from two data sources. Maximum and minimum air temperatures and rainfall were obtained from National Climatic Data Center (NOAA, http://www.ncdc.noaa.gov), while daily solar radiation was obtained from the NASA Prediction of Worldwide Energy Resource (POWER) - Climatology Resource for Agroclimatology (http://power.larc.nasa.gov). This long-term database also was used as a secondary source of maximum and minimum air temperatures to replace missing values from the

Table 1 Soil and climate characterization of locations used for the calibration/validation of the Agricultural Production Systems Simulator (APSIM)

			Climate description													Soil description	
				Tmax/Tmin (°C)*													
State	Location	Latitude, longitude	Rainfall (mm)*	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Series	Taxonomic classification
Calibration																	
IN	Columbia City‡	41.14, −85.49	938	−0.8/−8.5	0.9/−6.5	7.2/−1.0	14.9/5.1	21.5/11.0	26.5/15.7	28.4/17.6	27.6/16.8	23.6/12.6	16.4/6.9	8.7/1.2	1.5/−5.1	Boyer	Typic Hapludalfs
IN	West Lafayette†,‡	40.47, −87.01	978	0.3/−7.4	2.6/−5.1	9.0/0.3	16.7/6.5	22.9/12.7	27.8/17.2	29.6/19.0	28.9/18.0	24.7/13.8	17.9/8.2	9.9/2.0	2.5/−4.5	Drummer	Typic Haplaquolls
IN	Lafayette†,‡	40.30, −86.90	969	0.4/−7.2	2.4/−5.1	8.7/0.1	16.3/6.3	22.5/12.4	27.2/16.9	29.0/18.6	28.4/17.8	24.4/13.5	17.5/7.8	9.8/1.9	2.6/−4.4	Lauramie	Mollic Hapludalfs
																Octagon	Mollic Hapludalfs
IN	Butlerville‡	39.03, −85.52	1117	2.0/−5.3	3.9/−3.8	9.6/1.0	17.0/7.0	22.9/12.8	27.3/17.2	29.0/19.1	28.4/18.4	24.8/14.3	18.2/8.4	10.8/2.6	4.0/−3.0	Cobbsfork	Typic Glossaqualf
Validation																	
ND	Munich†	48.76, −98.34	452	−10.7/−19.7	−8.2/−17.5	−1.6/−10.9	10.1/−0.6	18.8/7.3	23.9/12.4	27.2/15.1	25.9/14.3	19.6/9.3	9.8/1.6	−1.2/−8.1	−8.7/−16.6	Tonka	Argiaquic Argialbolls
ND	Streeter†	46.73, −99.48	471	−7.9/−16.9	−5.7/−14.4	1.2/−7.8	11.2/−0.1	19.2/7.3	24.2/12.3	27.7/15.0	26.2/13.7	20.3/9.0	11.0/1.8	0.7/−6.7	−6.2/−14.1	Barnes	Udic Haploborolls
SD	Bristol†	45.27, −97.83	560	−7.6/−16.9	−5.1/−14.0	2.0/−6.9	12.0/0.9	20.0/8.3	25.2/13.4	28.4/15.8	26.9/14.5	21.2/9.8	12.0/2.8	1.8/−5.5	−5.5/−13.5	Buse	Udorthentic Haploboroll
SD	Huron†	44.39, −98.22	586	−5.2/−14.2	−2.6/−11.5	4.3/−5.1	13.1/1.6	20.6/8.7	25.6/13.9	29.2/16.4	27.7/14.9	22.3/10.2	13.4/3.2	3.5/−4.6	−3.5/−11.5	Dudley	Typic Natrustolls
SD	Highmore†	44.38, −100.28	472	−3.2/−12.3	−0.9/−9.9	5.5/−4.6	13.3/1.4	20.5/8.4	25.4/13.5	28.9/16.2	27.7/14.6	22.2/9.7	13.6/2.9	4.1/−4.6	−2.2/−10.4	Glenham	Typic Argiustoll
SD	Ethan†	43.65, −97.79	618	−4.3/−13.2	−1.7/−10.5	5.4/−4.1	13.8/2.4	21.0/9.3	26.1/14.5	29.2/16.9	27.8/15.4	22.8/10.6	14.2/3.8	4.5/−3.9	−2.5/−10.5	Houdek	Typic Haplustolls
NE	Crofton†	42.73, −97.50	729	−2.7/−11.7	−0.1/−9.0	6.9/−3.0	14.6/3.1	21.3/9.8	26.4/14.8	29.3/17.2	28.2/15.8	23.2/11.0	15.1/4.4	5.8/−3.0	−1.1/−9.1	Crofton	Typic Ustorthent
NE	Atkinson†	42.46, −98.65	626	−1.9/−10.9	0.5/−8.5	7.3/−3.0	14.5/2.8	21.1/9.4	26.0/14.6	29.2/17.3	27.9/15.8	23.1/10.9	15.1/4.1	6.0/−3.2	−0.6/−8.9	Pivot	Entic Haplustoll
NY	Ithaca†	42.46, −76.46	930	−2.4/−10.0	−1.0/−9.3	4.5/−4.3	12.3/2.2	19.4/8.0	24.2/12.9	26.2/15.3	25.1/14.6	21.0/10.8	13.9/4.9	6.8/−0.4	0.0/−6.4	Erie	Aeric Fragiaquepts
IA	Ames†	41.98, −93.69	925	−2.3/−10.6	0.3/−8.0	7.8/−1.2	15.9/5.1	22.2/11.6	27.4/16.8	29.9/19.1	29.0/17.8	24.0/12.7	16.5/6.4	7.4/−0.6	−0.1/−7.4	Clarion	Typic Hapludoll
IL	Dekalb†,‡	41.85, −88.85	897	−1.4/−9.6	0.8/−6.9	7.8/−0.6	15.8/5.6	22.4/12.0	27.7/16.8	29.7/18.7	28.7/17.6	24.3/13.1	17.1/7.4	8.6/1.0	0.9/−6.0	Flanagan	Typic Endoaquoll
NE	Mead‡	41.17, −96.46	743	−1.6/−10.1	0.9/−7.6	8.2/−1.4	16.0/4.6	22.3/11.2	27.3/16.2	30.1/18.5	29.2/17.3	24.1/12.4	16.3/6.0	7.2/−1.4	−0.1/−7.7	Tomek	Pachic Argiudolls
IA	Lucas†	40.92, −93.38	939	−0.5/−8.7	2.0/−6.3	9.4/0.0	17.0/6.0	22.8/12.2	27.8/17.4	30.4/19.8	29.7/18.6	24.8/13.4	17.6/7.2	8.8/0.4	1.5/−5.9	Grundy	Aquertic Argiudoll
IA	Wayne†	40.83, −93.25	934	−0.5/−8.7	2.0/−6.3	9.4/0.0	17.0/6.0	22.8/12.2	27.8/17.4	30.4/19.8	29.7/18.6	24.8/13.4	17.6/7.2	8.8/0.4	1.5/−5.9	Clarinda	Vertic Argiaquoll
NE	Douglas†	40.68, −96.19	789	−0.1/−8.6	2.4/−6.2	9.7/−0.3	17.1/5.6	22.9/11.9	27.8/16.9	30.7/19.4	30.0/18.3	24.7/13.2	17.4/7.0	8.6/−0.3	1.2/−6.4	Wymore	Aquertic Argiudolls
IN	Lafayette†	40.30, −86.90	969	0.4/−7.2	2.4/−5.1	8.7/0.1	16.3/6.3	22.5/12.4	27.2/16.9	29.0/18.6	28.4/17.8	24.4/13.5	17.5/7.8	9.8/1.9	2.6/−4.4	Lauramie	Mollic Hapludalfs

Table 1 (continued)

State	Location	Latitude, longitude	Rainfall (mm)*	Tmax/Tmin (°C)* Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Soil description: Series	Taxonomic classification
IL	Havana‡	40.30, −89.94	999	0.0/−7.8	2.4/−5.4	9.4/0.4	17.1/6.7	23.3/12.9	28.4/17.7	30.6/19.7	29.6/18.7	25.1/14.1	18.2/8.3	9.7/1.6	2.2/−4.9	Watseka	Typic Endoaquolls
NE	Lawrence†	40.29, −98.26	679	3.4/−5.8	5.8/−4.2	12.3/0.7	18.6/6.0	23.7/12.0	28.4/17.5	31.1/20.1	30.3/19.3	25.7/14.4	19.0/8.1	10.8/0.7	4.1/−4.4	Hastings	Udic Argiustolls
NJ	Adelphia‡	40.22, −74.25	1200	2.5/−4.6	3.8/−3.8	8.6/0.1	15.0/5.6	20.9/11.1	25.9/16.4	28.4/19.3	27.4/18.7	24.0/15.1	17.7/8.8	11.2/3.4	5.2/−1.5	Holmdel	Aquic Hapludults
IL	Urbana†,‡	40.08, −88.23	1024	0.0/−7.7	2.4/−5.3	9.2/0.4	16.9/6.6	23.2/12.9	28.1/17.6	30.1/19.4	29.3/18.3	24.9/14.0	18.0/8.3	9.8/1.8	2.3/−4.8	Flanagan	Typic Endoaquoll
IL	Brownstown‡	38.95, −88.96	978	3.2/−4.3	5.6/−2.3	11.6/2.4	18.7/8.3	24.3/14.2	28.6/18.7	30.3/20.5	29.9/19.7	25.9/15.4	19.8/9.7	12.1/3.5	5.2/−2.3	Cisne	Mollic Albaqualfs
CA	Davis‡	38.50, −121.70	453	13.2/3.8	14.1/4.1	16.5/5.2	19.7/7.1	24.3/10.7	29.0/14.2	32.3/16.4	31.4/15.7	29.2/14.6	24.0/11.6	17.3/7.0	13.0/4.0	Brentwood	Typic Xerochrepts
KY	Lexington‡	38.13, −84.50	1197	3.5/−3.8	5.5/−2.5	11.0/1.7	18.0/7.3	23.3/12.8	27.6/17.4	29.1/19.4	28.7/18.8	25.3/14.9	19.0/8.8	11.8/3.3	5.4/−1.7	Maury	Typic Paleudalfs
IL	Dixon Spring‡	37.45, −88.67	1246	4.7/−3.0	7.0/−1.2	12.7/3.3	19.5/9.0	24.8/14.7	29.0/19.3	30.6/21.0	30.3/20.3	26.5/16.1	20.6/10.2	13.1/4.2	6.5/−1.2	Grantsburg	Oxyaquic Fragiudalfs
VA	Gretna†,‡	36.93, −79.39	1141	6.8/−1.8	9.0/−0.7	14.1/2.9	20.2/8.2	25.0/13.4	28.8/18.0	30.2/20.2	29.2/19.5	26.0/15.9	20.6/9.5	14.2/4.2	8.6/0.0	Mayodan	Typic Hapludult
TN	Milan†	35.93, −88.71	1340	7.6/−0.4	10.0/1.2	15.2/5.3	21.1/10.2	25.9/15.6	29.7/19.9	30.9/21.6	30.8/21.1	27.5/17.4	22.2/11.4	15.2/5.7	9.5/1.2	Grenada	Oxyaquic Fraglossudalfs
																Vicksburg	Typic Udifluvents
OK	Muskogee†	35.74,−95.64	1074	7.5/−1.1	10.2/0.8	15.6/5.2	21.3/10.0	25.7/15.4	29.8/20.1	32.4/21.9	32.4/21.6	27.9/17.7	22.0/12.0	14.8/5.5	8.6/0.1	Parsons	Mollic Albaqualf
AR	Lewisville†	33.40, −93.58	1233	10.9/1.4	13.3/3.4	18.0/7.1	23.2/11.6	27.4/16.9	31.2/21.2	32.5/22.6	32.5/22.2	29.2/18.9	23.9/13.1	17.4/7.5	12.1/2.9	Bowie	Plinthic Paleudult
TX	Dallas†	32.58, −97.26	865	11.7/1.9	14.3/3.8	19.0/7.8	23.9/12.4	27.2/17.2	30.8/21.1	32.5/22.7	33.1/22.8	29.1/19.6	24.3/14.5	17.6/8.0	12.4/2.9	Houston Black	Udic Calciusterts
TX	Stephenville†	32.13, −98.20	756	11.5/1.3	14.0/3.2	18.9/7.4	23.9/11.9	26.8/16.6	30.2/20.6	32.1/22.1	32.5/22.1	28.5/18.7	23.7/13.8	17.1/7.3	12.0/2.1	Windthorst	Udic Paleustalfs
LA	Clinton†	30.51, −90.05	1224	15.4/5.8	17.4/7.4	20.9/10.4	24.7/14.0	28.1/18.5	30.4/22.0	30.9/23.1	31.0/23.0	29.0/20.8	25.2/15.5	20.5/10.8	16.6/7.2	Dexter	Ultic Hapludalf
TX	College Station†	30.36, −96.35	966	14.4/5.1	16.8/6.8	20.7/10.0	25.1/14.1	28.1/18.7	30.9/22.0	31.8/23.0	32.1/23.3	29.6/20.9	25.6/16.3	19.8/10.7	15.3/6.3	Norwood	Fluventic Eutrochrepts

*Rainfall, mean annual rainfall in long term; Tmax/Tmin, average maximum and minimum air temperatures in long term. The long-term data used for calculate Rainfall and Tmax/Tmin were based on period 1984 to 2014 for all locations.
†Switchgrass data were evaluated in this location.
‡*Miscanthus* data were evaluated in this location.

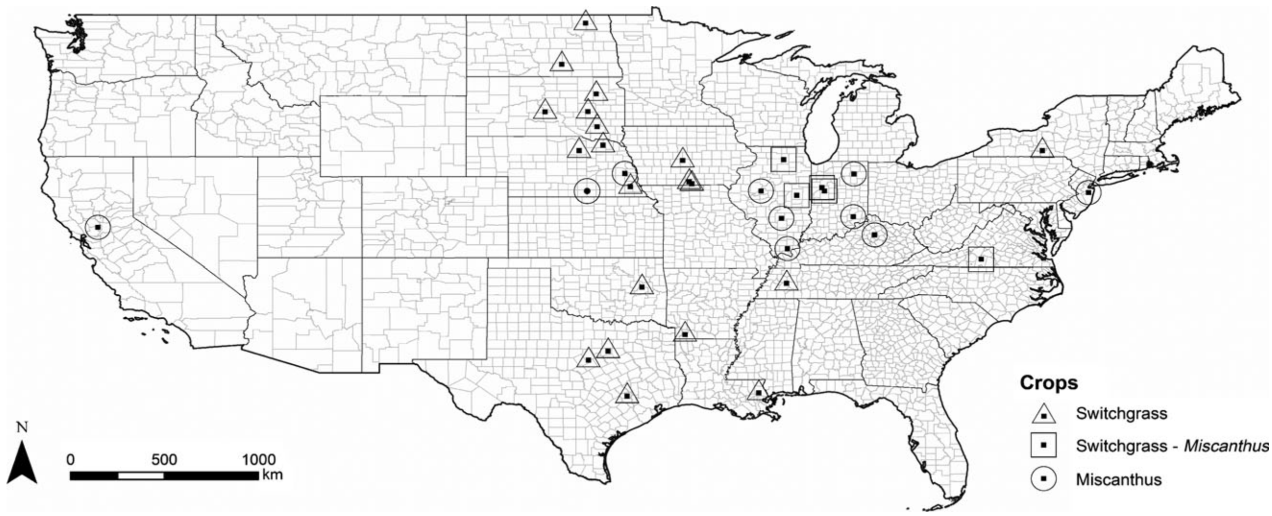

Fig. 1 Experimental sites included in the dry matter yield database for APSIM calibration/validation for switchgrass (△), switchgrass-*Miscanthus* (⊡) and *Miscanthus* (⊙). The data used for switchgrass validation were grouped in northern and southern locations. Northern locations: Indiana (IN), Illinois (IL), Tennessee (TN), Nebraska (NE), Iowa (IA), South Dakota (SD), New York (NY) and North Dakota (ND). Southern locations: Texas (TX), Virginia (VA), Oklahoma (OK), Louisiana (LA) and Arkansas (AR).

NOAA database. Interestingly, recent evaluations of the NASA-POWER solar radiation data indicate very good agreement with measured solar radiation data in areas with flat topography (White *et al*., 2011; Wart *et al*., 2013) and with maximum and minimum air temperatures across the US (White *et al*., 2008). Our evaluations demonstrated a similar fit for daily solar radiation (n = 59031 daily observations) and maximum and minimum air temperatures (n = 69505 daily observations) using measured data from 19 weather stations near the experimental locations used in this study (Fig. 2; Table S1). The number of air temperature data corrections/filled data was always lower than 2% for all variables.

Long-term monthly mean minimum air temperature ranged from −19.7 to 23.3 °C and the monthly mean maximum air temperature between −10.7 to 32.5 °C. The mean annual rainfall varied from 452 to 1340 mm for Munich, ND and Milan, TN respectively. A summary of climate information by location is reported in Table 1.

Soil parameterization

APSIM requires several soil parameters to adequately reflect the variability among locations (Probert *et al*., 1998; www.apsim.info). As the soil database of both the 7.3 and 7.5 release versions do not include the soils where these biophysical experiments were conducted, new APSIM soil profiles were created using the following process. First, dominant soil series were identified for each location based on data provided in the literature and in consultation with agronomists and local scientists (Table 1). Second, for each soil series actual soil data (texture, organic carbon [OC] and pH) were obtained from the National Cooperative Soil Survey Soil Characterization Database (NCSS, http://ncsslabdatamart.sc.egov.usda.gov) (see actual data in Table 2). Estimates of the drained upper limit (DUL) and the drained lower limit (LL) were estimated using the HYDRAULIC PROPERTIES CALCULATOR Software developed by Saxton & Rawls (2006) based on soil texture and OC data obtained from NCSS. The estimating equations reported by Saxton & Rawls (2006) were developed by correlation of an extensive data set (1722 samples) provided by the USDA/NRCS National Soil Survey Laboratory. As measured data of soil water parameters were not available for each evaluated location, the accuracy of the HYDRAULIC PROPERTIES CALCULATOR Software (Saxton & Rawls, 2006) to predict soil water parameters was gauged using the observed data of LL (mm mm^{-1}) and DUL (mm mm^{-1}) from soil series near the locations used in this study. An example of the soil parameterization for Drummer soil series at Water Quality Field Station, West Lafayette IN is presented in Table 2. A complete description of actual and estimated soil parameters used for the calibration/validation of APSIM are provided in the supplementary information for all location evaluated in this study (Table S5).

The APSIM modules were configured for soil N and C (APSIM *SoilN*), crop residue dynamics (APSIM *Surface Organic Matter*) and soil water (APSIM *SoilWat*). Actual OC (%) values were used for initialization (Table S5). To initialize the soil nitrogen pool for the simulations a 10-year simulation of previous management at the experimental locations (corn-soybean rotations), the location-specific climate and soil physical data were used. Crop growth data from these simulations were excluded from subsequent analysis.

For each soil, organic matter (OM, %, OM = OC*1.72; Dalgliesh & Foale, 1998); soil pH 1 : 5 (pH measured for a ratio of 1 part soil and 5 parts water solution according to GlobalSoilMap, 2012; estimated by Libohova *et al*., 2014); texture class; air dry (AD, mm mm^{-1}) corresponding to the moisture limit for dry evaporation of the soil; saturated volumetric water (SAT, mm mm^{-1}); bulk density (BD, Mg m^{-3}); hydraulic conductivity (ks, mm day^{-1}); total porosity (PO, 0–1 calculated as 1-BD/2.6); drainage coefficient (SWCON, day^{-1}) were estimated (Table S5).

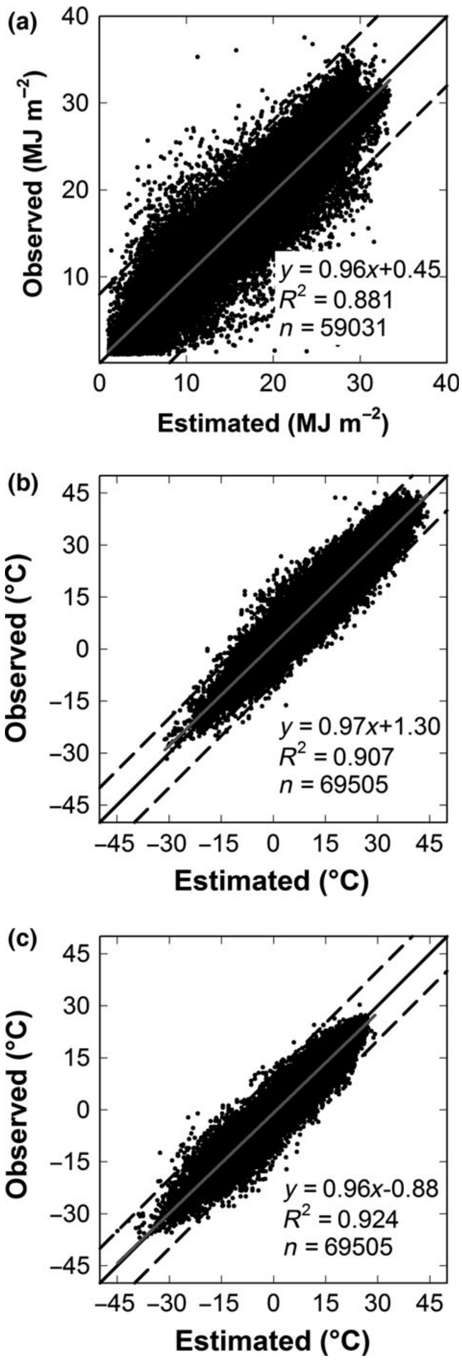

Fig. 2 Observed (a) daily incident solar radiation, (b) daily maximum air temperature and (c) daily minimum air temperature measured at 19 meteorological stations across United States plotted against daily data estimated from NASA-POWER. Solid black line represents the function $y = x$ (i.e. 1 : 1 relationship), dotted line represents ± 20% of 1 : 1 relationship and solid grey line represent the linear fit to the data.

Saturated water content was calculated from BD as described by Dalgliesh & Foale (1998). The parameter AD was estimated as 0.5 × LL in 0–0.15 m soil layer, 0.9 × LL in 0.15–0.3 m soil layer and equal to LL at depths >0.3 m (Cresswell *et al.*, 2009). The SWCON, the rate at which water drains, was estimated from DUL and BD (Jones & Kiniry, 1986). For each soil layer within each soil series the water extraction coefficient (KL, mm day^{-1}) was set at 0.08 mm day^{-1} (Robertson *et al.*, 1993a,b; Dardanelli *et al.*, 1997, 2004). The root exploration factor (XF, 0–1) was set to 1 for up to 1 m depth and then decreased exponentially to 0.6 at the maximum soil depth (Monti & Zatta, 2009). The maximum rooting depth was set according to maximum soil depth when there were no impediments to crop rooting. A complete description of actual and estimated soil parameters used for the calibration/validation of APSIM are provided in the supplementary information for each location (Table S5).

Initial soil water values were not available at most locations. Hence, an analysis of soil moisture data at sowing in some locations was performed. The data of seven climate monitoring stations (Lincoln, NE; Bedford and Lafayette, IN; Ithaca, NY; Crossville, TN; Bronte and Palestine, TX) were obtained from US Climate Reference Network (USCRN, http://www.ncdc.noaa.gov [Diamond *et al.*, 2013; Bell *et al.*, 2013]). The average of soil moisture at 0.2 m depth from these locations, from January to late April, was compared with the DUL of the 36 soils used in this study. With the exception of the TX sites, the initial soil water moisture in spring was always close to DUL. Based on this analysis, 100% of the initial soil water content was used at the onset of all simulations (not shown).

APSIM configuration

Without pre-existing APSIM modules for simulating switchgrass and *Miscanthus* we re-parameterized the APSIM *Lucerne* (Robertson *et al.*, 2002) and *Sugarcane* (Keating *et al.*, 1999) modules to simulate the growth of switchgrass (Table 4) and *Miscanthus* (Table 5) respectively. Switchgrass and *Miscanthus* simulations were undertaken using a daily time-step of the APSIM Version 7.5 and 7.3 respectively (Keating *et al.*, 2003; Holzworth *et al.*, 2014). After exhaustive and comparative analysis of plant modules, the re-parameterized APSIM *Lucerne* module best simulated switchgrass growth in terms of phenological and physiological functions (Table 4). Similarly, the phylogenetic proximity between *Saccharum officinarum* and *Miscanthus*, and similarity in physiology, phenology and growth, was the main justification for using the *Sugarcane* module as a starting point for re-parameterizing APSIM for predicting DM yield of *Miscanthus.* All the changes in the APSIM *Lucerne* and *Sugarcane* modules were implemented through changing parameterization in the initialisation file in extensible mark-up language (XML) format. Different management rules (i.e. sowing, harvesting, fertilization, irrigation, plant density, row spacing, etc.) were created according to practices used in the field and are reported in detail in the supplementary information for switchgrass (Table S3) and *Miscanthus* (Table S4). The harvesting rules were set to remove the biomass up to 0.03 m (Ojeda *et al.*, 2016). When the dates of management interventions were not available, local average dates for the application of these practices were used. A complete description of management practices used in the simulations is reported in the supplementary information (Tables S3 and S4 for switchgrass and

Table 2 Soil parameters for Drummer soil series at Water Quality Field Station, West Lafayette IN. Estimated data were obtained from actual data using pedotransfer functions

	Actual data					Estimated data									
	Texture							AD	LL	DUL	SAT	BD	ks	PO	SWCON
Depth cm	Sand %	Silt %	Clay %	OC %	pH 1 : 1	OM %	pH 1 : 5	mm mm^{-1}				Mg m^{-3}	mm day^{-1}	(0–1)	day^{-1}
0–23	15	56	30	2.49	6.0	4.3	5.8	0.095	0.189	0.361	0.483	1.24	165	0.52	0.277
23–43	12	56	32	0.96	6.3	1.7	6.2	0.180	0.200	0.371	0.490	1.22	152	0.53	0.270
43–71	9	60	31	0.71	6.6	1.2	6.5	0.194	0.194	0.373	0.493	1.21	165	0.53	0.268
71–94	14	62	23	0.34	7.2	0.6	7.1	0.152	0.152	0.342	0.478	1.25	232	0.52	0.292
94–109	65	26	9	–	8.0	–	8.0	0.075	0.075	0.174	0.441	1.35	1317	0.48	0.575
109–190	64	29	6	–	8.0	–	8.0	0.075	0.075	0.177	0.441	1.35	1292	0.48	0.565
190–244	41	41	18	–	8.1	–	8.1	0.126	0.126	0.269	0.447	1.33	439	0.49	0.372
244–330	42	42	16	–	8.1	–	8.1	0.126	0.126	0.267	0.446	1.33	445	0.49	0.375

OC, organic carbon; pH (1 : 1), pH in a 1 : 1 suspension of soil in water; pH (1 : 5), pH in a 1 : 5 suspension of soil in water; OM, organic matter; AD, air dry; LL, lower limit; DUL, drained upper limit or field capacity; SAT, saturated volumetric water content; ks, hydraulic conductivity; BD, bulk density; PO, total porosity; SWCON, drainage coefficient.

Miscanthus, respectively). The used model output from each simulation was crop DM yield (kg ha^{-1}). The simulations in West Lafayette IN included the additional analysis of LAI as another model output. The cultivars used in the field experiments were created as two generic switchgrass genotypes (generic lowland and generic upland) and one *Miscanthus* genotype (generic) differing in thermal time requirements needed to attain specific phenological stages (Table S6).

Sensitivity analysis

A sensitivity analysis enables users to determine the responses of key model outputs (*e.g.*, harvestable biomass, hereafter DM yield) to variations in selected input parameters. Hence, as part of model calibration, a sensitivity analysis of the APSIM *Lucerne* and *Sugarcane* module's to plant and soil parameters (Table 3) was performed using the one-at-a-time method to evaluate parameter influence on LAI and DM yield. Three soil datasets were chosen to represent a range in relevant soil textures (silty, loamy and sandy). We used these soils to analyse the sensitivity of the model parameters through a large range of plant available water capacity (PAWC).

Based on an exhaustive review of the literature, and field-measured data, and in order to adequately predict the growth of switchgrass and *Miscanthus* with the APSIM *Lucerne* and *Sugarcane* modules, the most sensitive plant parameters for switchgrass (Fig. 3; Fig. 6) and *Miscanthus* (Fig. 3; Fig. 9) were identified (Tables 4 and 5 for switchgrass and *Miscanthus*, respectively). Thereafter, in extensible mark-up language (XML) format, these parameters were modified (Tables 4 and 5 for switchgrass and *Miscanthus*, respectively). In all cases, the modified parameters were calculated as an average of reported values in the literature or field measurement based on the range of each parameter. For all locations, we used the same values of parameters to simulate the DM yield in the re-parameterized modules. We followed the same parameterization process for both crops, although there were more sensitive parameters for switchgrass than for *Miscanthus*, which explain the differences in the number of parameters listed in Tables 4 and 5. It should be noted that we only showed the modified parameters, since default (original) values might be easily obtained from the XML file available in the free APSIM version.

In the APSIM *Sugarcane* module crop growth is divided into two sections, plant and ratoon crop. The parameters in the plant and ratoon crop sections determine the crop growth for the first and second harvests onwards. Hence, the model modifications were made in both sections of XML file (plant and ratoon crop). To assess potential errors in soil datasets, after plant model modifications, a sensitivity analysis was undertaken for PAWC (Fig. 4a for switchgrass and Fig. 4b for *Miscanthus*). The maximum variation (%) in the parameters that determine the maximum PAWC in the soil - AD, LL, DUL and SAT - was determined based on the 36 soils used in this study (Table S2). Therefore, for the sensitivity analysis AD, LL, DUL and SAT were modified in ±29%, ±23%, ±10% and ±5%, respectively, in order to provide realistic boundaries. Second, sensitivity of KL, XF and initial OC was evaluated by modifying the range ±50% of initial values (Fig. 4c,e,g for switchgrass and Fig. 4d, f, h for *Miscanthus*). Using the same approach explained previously, the maximum pH variation (%) was determined (Table S2). Model sensitivity to pH change was evaluated by increasing and decreasing soil pH by 14% of the actual soil values of switchgrass (Fig. 4i) and *Miscanthus* (Fig. 4j). The total number of simulations necessary to complete the sensitivity analysis of soil parameters was 958.

Re-parameterization of switchgrass plant module

Crop phenology in APSIM is controlled by the sum of heat units from sowing to maturity. Accordingly, the parameter *y_tt* (thermal time requirements needed to attain specific phenological stages) was set to the growth habit of switchgrass (Kiniry *et al.*,

Table 3 Plant and soil parameters evaluated through the sensitivity analysis for the APSIM re-parameterization to simulate the DM yield of switchgrass and *Miscanthus* with their description, acronym/abbreviation. Note that some parameters vary according with the crop

		Acronym/Abbreviation	
	Definition	Switchgrass	*Miscanthus*
Plant	Thermal time calculation	*y_tt*	*y_tt*
	Stem reduction effect on phenology	*stage_stem_reduction_harvest*	–
	Radiation use efficiency	*y_rue*	*y_rue*
	Transpiration efficiency coefficient	*transp_eff_cf*	*transp_eff_cf*
	Temperature response of photosynthesis – RUE*	*y_stress_photo*	*y_stress_photo*
	Water stress on phenology	*y_swdef_leaf*	*swdf_pheno_limit*
		y_swdef_pheno	*y_swdef_pheno*
		y_swdef_pheno_flowering	*y_swdef_pheno_flowering*
		y_swdef_pheno_start_grain_fill	*y_swdef_pheno_start_grain_fill*
	Water stress on photosynthesis	–	*swdf_photo_limit*
	Water stress during photosynthesis to leaf senescence rate	–	*sen_rate_water*
	Frosting stress	*frost_fraction*	–
	Extinction coefficient	*y_extinct_coef*	*extinction_coef*
	Biomass partitioning	*ratio_root_shoot*	*ratio_root_shoot*
Soil	Plant available water capacity	*PAWC*	*PAWC*
	Water extraction coefficient	*KL*	*KL*
	Root exploration factor	*XF*	*XF*
	Initial organic carbon	*OC*	*OC*
	pH	*pH*	*pH*

*RUE, radiation use efficiency.

2005). Similarly, the *stage_stem_reduction_harvest* parameter was modified so that, after harvest, switchgrass starts a new regrowth. In order to achieve this initial point of growth, *stage_stem_reduction_harvest* was reduced from 4 to 3 (Table 4).

The LAI and, hence, DM yield in APSIM are defined directly by the RUE and the transpiration efficiency coefficient (Kc) parameters both fixed in each phenological stage. Modifications of the physiological parameters reported elsewhere for the APSIM *Lucerne* module (Dolling *et al*., 2005; Brown *et al*., 2006; Chen *et al*., 2008) were also used here to simulate switchgrass DM yields. After sensitivity analysis, RUE (coded by *y_rue*; Madakadze *et al*., 1998; Kiniry *et al*., 1999, 2012; Heaton *et al*., 2008; Jain *et al*., 2010; Trybula *et al*., 2014) and Kc (coded by *transp_eff_cf*; Byrd & May, 2000) were set based on switchgrass values obtained in the literature (Table 4). For all locations, we used the same RUE and Kc value. In addition, two other parameters (the temperature response of photosynthesis, *y_stress_photo*, and the extinction coefficient, *y_extinct_coef*) directly associated with DM yield were modified as follows. The temperature response of photosynthesis was modified based on previous corn studies (Andrade *et al*., 1993; Louarn *et al*., 2008) validated for switchgrass (Grassini *et al*., 2009) (Table 4). Similarly, *y_extinct_coef* was modified based on the differences in leaf structure between lucerne vs. switchgrass (Kiniry *et al*., 1999; Trybula *et al*., 2014).

Re-parameterization of Miscanthus plant module

Several researchers have reported wide differences in RUE values for *Miscanthus*. Kiniry *et al.* (2012) reported a low value of RUE (1.3 g MJ^{-1}) in central TX. In contrast, the same authors reported a value of 3.7 g MJ^{-1} in the north-eastern MO whereas Heaton *et al.* (2008) reported a high value of RUE (4.1 g MJ^{-1}) in IL. Other studies reported RUE values of 2.2, 2.4 and 2.3–3.0 g MJ^{-1} in Italy (Cosentino *et al*., 2007), UK (Clifton-Brown *et al*., 2001) and IL (Dohleman & Long, 2009), respectively. Hence, given these discrepancies in RUE values among studies, the parameter *y_rue* was modified from 1.8 g MJ^{-1} to 3.0 g MJ^{-1} for all phenological stages (Table 5). This used value of RUE was calculated from these studies as an average of the ratio between accumulated yield (from emergence to peak biomass) and total annual incident radiation. For all locations, we used the same RUE value (3.0 g MJ^{-1}).

The light extinction coefficient (coded by *y_ extinct_coef*) through the leaf cover of the crop provides a measurement of the absorption of light by leaves (Zub & Brancourt-Hulmel, 2010). *Miscanthus* achieves *y_ extinct_coef* values between 0.45 (Trybula *et al*., 2014) to 0.68 (Clifton-Brown *et al*., 2000). Based on the insensitivity to the changes of this parameter in the range reported in the literature (Fig. 3d), the *y_ extinct_coef* default value for *Miscanthus* (0.38) was unchanged. *Miscanthus* partition biomass has been parameterized for the WIMOVAC model using data from Beale & Long (1997) and has been validated using data from European studies (Miguez, 2007). Based on the data collected by Burks (2013) and Trybula *et al.* (2014) in West Lafayette IN, the *ratio_root_shoot* parameter was modified in APSIM for all phenological stages (Table 5). These authors measured the *Miscanthus* aboveground and root biomass in different crop growth stages. Therefore, we used these data to re-parameterize the *ratio_root_shoot* into the *Sugarcane*

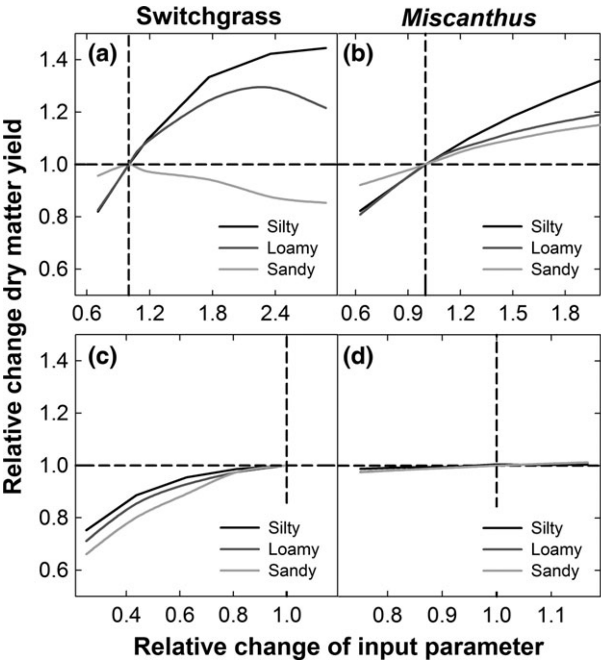

Fig. 3 Relative change in predicted dry matter yield of switchgrass and *Miscanthus* vs. relative change of plant parameters for three contrasting soil textures. Switchgrass and *Miscanthus* were modelled using APSIM *Lucerne* and APSIM *Sugarcane* modules, respectively. The plant parameters analysed were: *y_rue*, radiation use efficiency (a, b) and *y_extinct_coef*, extinction coefficient (c, d). The value 1 on the *x*-axis corresponds to the model default values used in the sensitivity analysis. Broken lines indicate the baseline parameter and no changes in dry matter yield, respectively.

APSIM module for emergence, juvenile and flowering stages. A complete description of *ratio_root_shoot* values obtained by these authors are provided in the supplementary information (Table S7).

Evaluation of model performance

Initially, model performance was visually assessed by comparing scatter plots of observed values in the *y*-axis vs. modelled values in the *x*-axis (Piñeiro *et al.*, 2008). When multiple data points were available for a particular treatment in an experiment, standard deviations are included as an estimate of error. The evaluation of model performance described in Tedeschi (2006) and Kobayashi & Us Salam (2000) were used to statistically evaluate model performance. The parameters used were: observed and modelled mean and standard deviation of the DM yield, the concordance correlation coefficient (CCC), and mean square error (MSE). The CCC integrates precision through Pearson's correlation coefficient, which represents the proportion of the total variance in the observed data that can be explained by the model, and accuracy by bias which indicates how far the regression line deviates from the concordance ($y = x$) line. Similarly, the MSE was partitioned into bias (SB, %, the bias of the simulation from the measurement) and mean square variation (MSV, %, the difference between the simulation and the measurement with respect to the deviation from the means), using IRENE software (Fila *et al.*, 2003). Bias and MSV are orthogonal and, consequently, can be analysed independently (Kobayashi & Us Salam, 2000). Model calibration was deemed complete when the CCC and SB were higher than 0.7 and <30%, respectively, for the LAI and DM yield of both crops.

In both crops, the growth period from sowing was simulated including the establishment phase, during which time rhizome biomass, root depth, and DM yield are increasing, and the post-establishment phase, in which perennial organs and root system are fully developed and the DM yield is fairly constant. This is influenced more by variation in weather than changes in plant establishment/underground organ development. However, only the observed DM yield from the post-establishment phase was included in this analysis to evaluate the accuracy of the model to predict DM yield with the established crop. The duration of the establishment phase varied from two to four years, depending on the experimental site (Tables S3 and S4). For switchgrass validation, the data sets were grouped by northern locations (IN, Indiana; IL, Illinois; TN, Tennessee; NE, Nebraska; IA, Iowa; SD, South Dakota; NY, New York; ND, North Dakota) and southern locations (TX, Texas; VA, Virginia; OK, Oklahoma; LA, Louisiana; AR, Arkansas). The same grouping was not applied to *Miscanthus*, because DM yields in southern US locations are extremely low and difficult to find in the literature. Therefore, the capability of APSIM to simulate the *Miscanthus* DM yield was not evaluated in southern US locations.

Results

Switchgrass

The most sensitive parameters of plant module were RUE and the light extinction coefficient coded by *y_rue* and *y_ extinct_coef* parameters, respectively. The sensitivity of the model to the modification of these parameters (Fig. 3a,c) was high in the selected soils. The largest change in DM yield (29% and 44%) occurred when *y_rue* was increased from 1.7 to 4 g MJ^{-1} and 4.9 g MJ^{-1} in the loamy and silty soils, respectively (Fig. 3a). In contrast, increasing *y_rue* to 4.9 g MJ^{-1} reduced switchgrass DM yield by ~15% in the sandy soil (Fig. 3a). The trend in DM yield to decreased *y_extinct_coef* was similar for these soils with declines 5–11% and 25–34% when *y_extinct_coef* was decreased from 0.8 to 0.5 and 0.8 to 0.2, respectively (Fig. 3c).

The sensitivity analysis carried out to identify possible effects of changing soil parameters in the re-parameterized model (Fig. 4) on switchgrass DM yields also showed soil-specific responses with the greatest responses in DM yield occurring in the sandy soil. For example, when PAWC was decreased, predicted DM yield declined 1%, 7% and 11% for silty, loamy and

Table 4 Parameterization of APSIM *Lucerne* plant module for switchgrass simulation. List of the modified parameters with their section into the XML file, definitions, acronym, units, default (original), used values (modified) and range of values found in the literature and references

Definition	Acronym	Units	Default value/s											Used values											Range/ References
Crop phenology																									
Thermal time calculation	*x_temp*	°C	1	5	10	15	30	40						12	25	45									Kiniry *et al.*, 2005
	y_tt	°Cd	0	3	6.5	10	25	0						0	13	0									
Stem reduction effect on phenology	*stage_code*	0–11	1	2	3	4	5	6	7	8	9	10	11	1	2	3	4	5	6	7	8	9	10	11	
	stage_stem_ reduction_ harvest	0–11	1	2	3	4	4	4	4	4	4	4	11	1	2	3	3	3	3	3	3	3	3	11	
Photosynthesis, biomass growth and partition																									
Stage dependent RUE*,†	*stage_code*	0–11	1	2	3	4	5	6	7	8	9	10	11	1	2	3	4	5	6	7	8	9	10	11	**1.7–4.9**/Madakadze *et al.*, 1998 Kiniry *et al.*, 1999, 2012 Heaton *et al.*, 2008 Jain *et al.*, 2010
	y_rue	g MJ^{-1}	0	0	0.7	0.7	0.5	0.4	0.1	0.1	0	0	0	0	0	1.7	1.7	1.7	1.7	1.7	1.7	0	0	0	Trybula *et al.*, 2014
Stage dependent transpiration efficiency coefficients,†	*stage_code*	0–11	1	2	3	4	5	6	7	8	9	10	11	1	2	3	4	5	6	7	8	9	10	11	Byrd & May, 2000
	transp_eff_cf	Pa	0	0	0.006	0.006	0.005	0.003	0.001	0	0	0	0	0	0	0.0055	0.0055	0.0055	0.0055	0.0055	0	0	0	0	
Temperature response of photosynthesis - RUE	*x_ave_temp*	°C	0	8	20	25	40							0	6	9	12	17	21	42					Andrade *et al.*, 1993 Louarn *et al.*, 2008
	y_stress_photo	0–1	0	1	1	1	0							0	0	0.2	0.4	0.7	1	0					Grassini *et al.*, 2009
Extinction coefficient	*x_row_spacing*	mm	100	1000										100	1000										**0.20–0.55**/Kiniry *et al.*, 1999
	y_extinct_coef	0–1	0.8	0.8										0.5	0.5										Trybula *et al.*, 2014

*RUE, radiation use efficiency.

†The modification shown in this table made in the plant section for transpiration efficiency coefficient also was made in the lucerne regrowth section of the XML file. The meaning of bold values is the range of parameters values found in the literature.

Table 5 Parameterization of APSIM *Sugarcane* module plant module for *Miscanthus* simulation. List of the modified parameters with their section into the XML file, definitions, acronym, units, default (original), used values (modified) and range of values found in the literature and references

Definition	Acronym	Units	Default value/s						Used value/s						Range/References
Plant and ratoon crop*															
Stage dependent RUE†	*stage_code*	0–6	1	2	3	4	5	6	1	2	3	4	5	6	**1.3–4.1**/Clifton-Brown *et al.*, 2001 Cosentino *et al.*, 2007 Heaton *et al.*, 2008 Dohleman & Long, 2009 Jain *et al.*, 2010 Kiniry *et al.*, 2012 Trybula *et al.*, 2014
	rue	g MJ^{-1}	0	0	1.8	1.8	1.8	0	0	0	3	3	3	0	
Biomass partitioning	*stage_code*	0–6	1	2	3	4	5	6	1	2	3	4	5	6	**0.2–0.8**/Burks, 2013 Trybula *et al.*, 2014
	ratio_root_shoot	0–1	0	0	0.2	0.2	0.1	0	0	0	0.85	0.37	0.22	0	

*The modifications shown in this table made in the plant section into the XML file also were made in the ratoon crop section.
†RUE, radiation use efficiency.

sandy soils, respectively (Fig. 4a). When PAWC was increased, the DM yield was enhanced 3%, 4% and 5% for silty, loamy and sandy soils, respectively (Fig. 4a). The highest DM yield response to changes in XF, KL and pH also occurred in the sandy soil (13%, 14% and 21%, respectively; Fig. 4e,c,i). By comparison, the model was less sensitive (<4%) to the changes in the initial OC (Fig. 4g).

The model with the default settings demonstrated a poor ability to simulate LAI and DM accumulation of switchgrass. Summary statistics comparing observed and modelled LAI from original and modified model parameters at the Water Quality Field Station in West Lafayette IN demonstrated the improvement in LAI predictions, as indicated by the increased CCC values (0 to 0.81) and a reduction in the SB (93 to 30%) (Fig. 5a; Table 6). Similarly, and as expected, when modified plant parameters (Fig. 6; Table 4) were introduced into the APSIM *Lucerne* module, prediction of switchgrass DM yield at the same location was improved, as indicated by the increase CCC (0.11 to 0.96) and the reduction in SB (57 to 4%) (Table 6).

The APSIM *Lucerne* module showed excellent accuracy for predicting the accumulated DM yield at IN locations used for switchgrass model calibration (Fig. 10a) as evidenced by the values of 0.93 for the CCC and 0% for the SB (Table 7). The APSIM *Lucerne* module also predicted DM yields when validated using yield data from trials conducted at northern locations (Fig. 11a), but model accuracy at southern locations was unsatisfactory. In fact, the CCC = 0.95 from comparisons using data from northern locations contrasted with the CCC = 0.01 for comparisons using data from southern locations (Table 7). Remarkably, SBs obtained for northern and southern locations were similar, 0 vs. 2%. The observed switchgrass DM yield during validation ranged from 5329 kg DM ha^{-1} in SD to 10668 kg DM ha^{-1} in IN, with the average discrepancy in DM yield being 1%. The modelled DM yield ranged from 1391 kg ha^{-1} in VA to 10786 kg ha^{-1} in TN. The better DM yield predictions in the northern locations were in IL, TN, NE, IA and SD. In contrast, in NY, IN, and ND the switchgrass DM yield was simulated with less precision (Table 7). By comparison, the modelled DM yields at southern locations were, on average, 10% less than observed values. When data were clustered by ecotype at northern locations, the DM yield was better predicted for upland ecotypes (0.96 for the CCC and 0% for the SB) than for lowland ecotypes (0.64 for the CCC and 9% for the SB). The variation of DM yield was well predicted by the re-parameterized model irrespective of stage of establishment of the crop.

Better estimates of soil water parameters (LL and DUL) were obtained from the HYDRAULIC PROPERTIES CALCULATOR Software (Saxton & Rawls, 2006) for northern locations (CCC = 0.92–0.98 and SB = 0–14%) than for southern locations (CCC = 0.75–0.92 and SB = 0–37%) (Table 8; Fig. 7).

Results of regression analysis of observed DM yields on accumulated annual rainfall revealed a poor fit at southern US locations (R^2 = 0.18 and slope regression −4.43; Fig. 8a). In contrast, the rainfall regression at northern locations showed a greater R^2 value (0.43) than the southern locations, and a positive slope (6.18) (Fig. 8b).

Miscanthus

As with the *Lucerne* plant module, the most sensitive parameter of the *Sugarcane* plant module was *y_rue*. However, unlike *y_rue*, the model was not sensitive to changes in *y_extinct_coef* (Fig. 3d). Model sensitivity to modification of *y_rue* (Fig. 3b,d) varied depending on

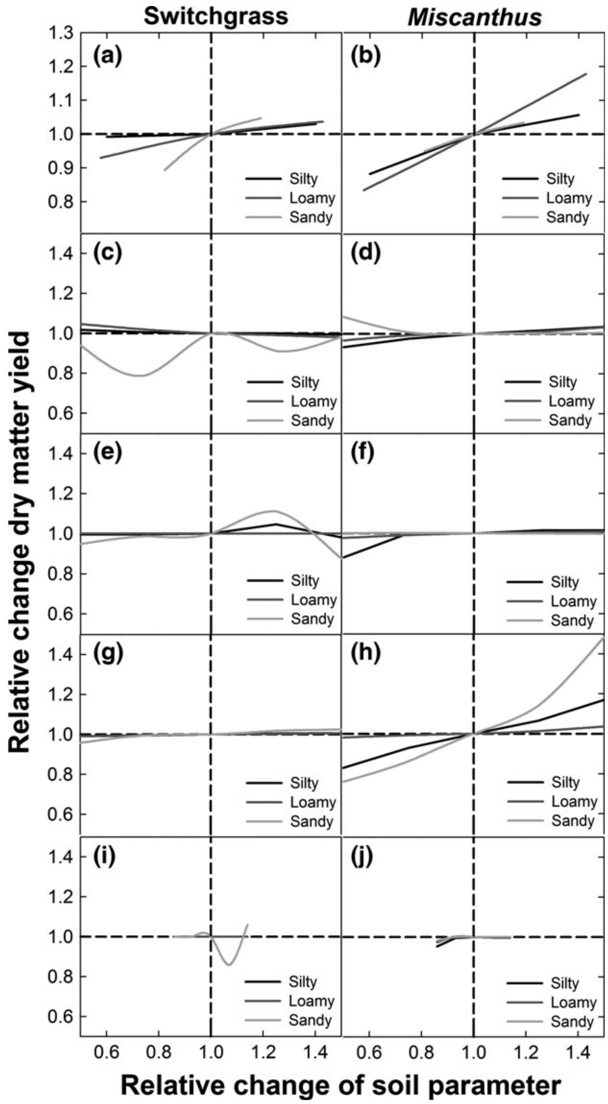

Fig. 4 Relative change in dry matter yield of switchgrass and *Miscanthus* vs. relative change of soil parameters using APSIM *Lucerne* and APSIM *Sugarcane* modules, respectively, for three contrasting soil textures. The soil parameters analysed were PAWC, plant available water capacity (a, b); KL, water extraction coefficient (c, d); XF, root exploration factor (e, f); OC, initial organic carbon (g, h) and pH (i, j). The value 1 on the *x*-axis corresponds to the default values used in the sensitivity analysis. Broken lines indicate the baseline parameter and no changes in dry matter yield, respectively.

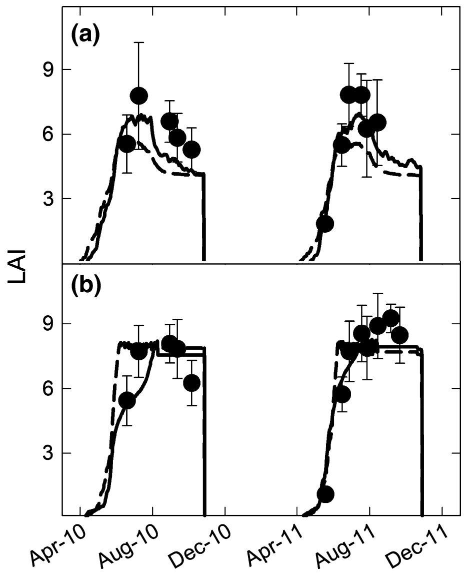

Fig. 5 Modelled pre- (---), post-APSIM modification (—) and observed (●) LAI of (a) switchgrass and (b) *Miscanthus* at Water Quality Field Station (West Lafayette, IN) during two seasons. Vertical bars represent the standard deviation of observed values.

soil type. The largest change in DM yield (increment of 15–32%) occurred when *y_rue* was increased from 1.8 to 4 g MJ^{-1} (Fig. 3b). Reducing *y_rue* from 1.8 to 1.25 g MJ^{-1} resulted in 8–19% lower DM yields when compared to initial model conditions (Fig. 3b).

The sensitivity analysis carried out to identify possible effects of soil parameters (Fig. 4) on *Miscanthus* DM yield showed differential responses depending on soil type and parameter. When PAWC was increased, changes in DM yield were higher for the loamy soil (18%) than for the silty and sandy soils (6% and 3% respectively; Fig. 4b). Similarly, when PAWC was decreased, the reductions in DM yield were greater for the loamy soil (17%) than for the silty and sandy soils (12% and 5%, respectively; Fig. 4b). When initial OC was increased by 50% from default values, predicted increases in DM yield on sandy soil (48%) were higher than the silty soil (17%) and the loamy soil (4%; Fig. 4h). In contrast, the model exhibited low sensitivity of DM yield to soil pH, KL and XF with changes in DM yield predicted to be no >5%, 9% and 12% for the respective parameters (Fig. 4j,d,f).

The original APSIM *Sugarcane* model with the default plant parameters could not accurately predict *Miscanthus* LAI and accumulated DM yield. Summary statistics comparing observed to predicted LAI with the re-parameterized model using data from the Water Quality Field Station in West Lafayette, IN demonstrated improvement in LAI predictions as indicated by the high CCC (0.69) and low SB (<30%) (Fig. 5b; Table 9). Similarly, and as expected, when modifications of plant parameters (Fig. 9; Table 5) were introduced into the model, the prediction of *Miscanthus* DM yield, at the same location was improved as indicated by the excellent CCC (0.94) and low SB (<30%) (Table 9).

The re-parameterized APSIM *Sugarcane* module showed excellent accuracy for predicting *Miscanthus*

Table 6 Summary statistics indicating the cumulative improvement that resulted from re-parameterization of the APSIM *Lucerne* model for predicting LAI (n = 11) and dry matter yield (n = 20) of switchgrass at Water Quality Field Station, West Lafayette, IN. The parameters modified were *y_tt*, thermal time requirements needed to attain specific phenological stages; *y_rue*, radiation use efficiency; *transp_eff_cf*, transpiration efficiency coefficient; *y_stress_photo*, temperature response of photosynthesis and *y_extinct_coef*, extinction coefficient. CCC, SB and MSV are the concordance correlation coefficient, bias of the simulation from the measurement and mean square variation, respectively

	Original model	*y_tt*	*y_rue*	*transp_eff_cf*	*y_stress_photo*	*y_extinc_coef*
LAI						
Mean (Observed)	6.1	6.1	6.1	6.1	6.1	6.1
Mean (Modelled)	0.0	4.7	5.2	5.4	5.5	5.5
SD (Observed)	1.7	1.7	1.7	1.7	1.7	1.7
SD (Modelled)	0.0	0.9	1.6	1.4	1.3	1.5
Testing parameters						
CCC	0.00	0.66	0.60	0.67	0.76	0.81
SB (%)	93	60	26	23	23	30
MSV (%)	7	40	74	77	77	70
Dry matter yield (kg ha^{-1})						
Mean (Observed)	5908	5908	5908	5908	5908	5908
Mean (Modelled)	411	2324	5503	7435	6263	6154
SD (Observed)	4939	4939	4939	4939	4939	4939
SD(Modelled)	1774	1920	4094	4929	4543	4530
Testing parameters						
CCC	0.11	0.65	0.85	0.94	0.96	0.96
SB (%)	57	58	3	45	7	4
MSV (%)	43	42	97	55	93	96

DM yield at IN locations used for model calibration (Fig. 10b) as evidenced by the values of 0.92 and 13% for the CCC and SB respectively (Table 10). The model validation was acceptable for most locations (0.65 and 0% for CCC and SB, respectively; Fig. 11b). However, the model accuracy at KY and NJ was unacceptable as indicated by the low CCC values of 0.38 and 0.46, respectively (Table 10). However, the SB obtained during validation was similar and <30%. The observed DM yield of *Miscanthus* for validation ranged from 8398 kg DM ha^{-1} in VA to 33980 kg DM ha^{-1} under irrigated conditions in CA (Fig. 11b). The modelled DM yield for calibration was 9% higher than observed DM yield. This difference, however, was negligible (0.5%) when compared to the observed and modelled DM yield association done for validation (Table 10). The modelled DM yield ranged from 13883 kg DM ha^{-1} in VA to 20518 kg DM ha^{-1} in NE.

Discussion

The main objective of this study was to evaluate the ability of APSIM to simulate the growth and DM yields of switchgrass (using the re-parameterized *Lucerne* module) and *Miscanthus* (using the re-parameterized *Sugarcane* module) at several locations across the US. The modelling approach was based on an exhaustive sensitivity analysis of plant and soil parameters using the one-at-a-time method followed by a detailed model calibration using field data from experiments in IN, and ending with a model validation using data from numerous US locations. Results indicate that these re-parameterized APSIM *Lucerne* and *Sugarcane* modules can accurately simulate growth and yield of switchgrass and *Miscanthus* respectively. Further considerations, specific to each crop, are discussed below.

Switchgrass

The original APSIM *Lucerne* module was developed and extensively tested in many environments for its ability to predict the phenology and DM yield of lucerne (Robertson *et al.*, 2002; Dolling *et al.*, 2005; Chen *et al.*, 2008; Pembleton *et al.*, 2011; Moot *et al.*, 2015; Ojeda *et al.*, 2016). However, in its original format with thermal parameters for a C3 species, the module is not able to adequately simulate switchgrass DM yield. Therefore, several modifications in plant module parameters were needed to improve the prediction of switchgrass DM yield. The range of modelled DM yield in this study for northern locations (5392 to 10 668 kg ha^{-1}) was coincident with modelled DM yields of the upland ecotype (Wang *et al.*, 2015) in the marginally saline soil of northeast Fort Collins, CO (5200 to 9600 kg ha^{-1}), as well as with the observed DM yield described by Schmer *et al.* (2008) on marginal cropland on ten farms in ND, SD

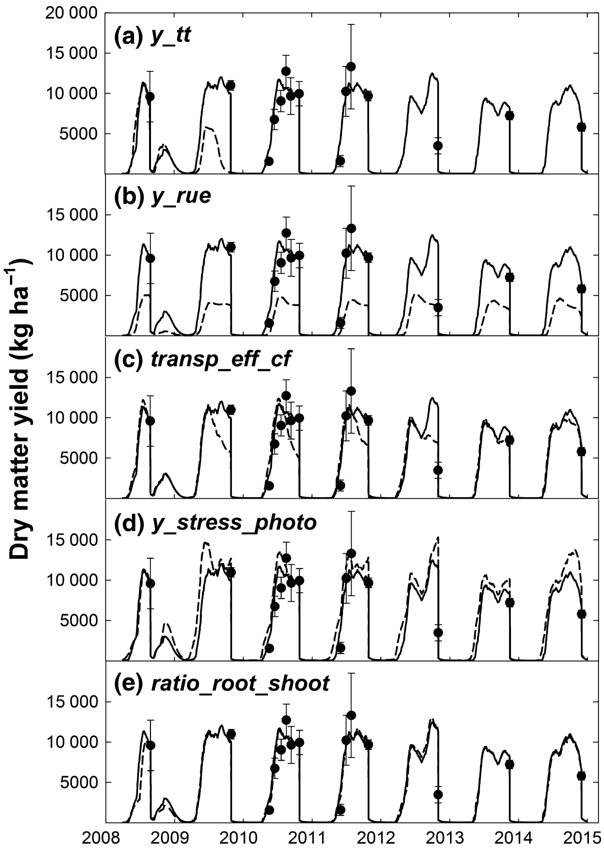

Fig. 6 Modelled pre- (---), post-APSIM *Lucerne* modification (—) and observed dry matter yield (●) of switchgrass cultivar Shawnee at Water Quality Field Station (West Lafayette, IN). The modified parameters shown in each panel are *y_tt*, thermal time requirements needed to attain specific phenological stages (a); *y_rue*, radiation use efficiency (b); *transp_eff_cf*, transpiration efficiency coefficient (c); *y_stress_photo*, temperature response of photosynthesis (d) and *ratio_root_shoot*, ratio root/shoot (e). The effect on dry matter yield was only due to the modification of each individual parameter. Vertical bars represent the standard deviation of observed values.

and NE (5200 to 11 100 kg ha^{-1}) and by Wullschleger *et al.* (2010) for 25 upland cultivars in the northern US.

The re-parameterization was based on sensitivity of DM yield when parameters were modified to values obtained in published studies (Table 4). In addition, differential effects of soil parameters on switchgrass DM yield were observed (Fig. 4). Soil water availability is one of the key soil parameters that explained most of the differences in switchgrass growth and yield (Fig. 4a). Similarly, the low PAWC due to high sand contents in the soil (Saxton & Rawls, 2006) reduced the canopy expansion decreasing the light interception and photosynthesis, thus, reduced plant growth (Durand *et al.*, 1995) in tall fescue. In addition, our results showed highest sensitivity of DM yield to parameter changes in the sandy soil that had the lowest PAWC. Although the re-parameterized model substantially improved the prediction of DM yield at northern locations, a poor DM yield prediction at southern US locations was found (Figs 10 and 11a). This poor validation was associated with difficulty in accurately estimating PAWC at southern locations (Fig. 7), specifically estimates of LL and DUL by the HYDRAULIC PROPERTIES CALCULATOR Software (Saxton & Rawls, 2006) (Table 8). This was evidenced by the statistical analysis performed on observed and estimated LL and DUL at ten soil series near selected southern and northern locations evaluated in this study (Table 8). For example, the over and under estimation of PAWC at OK and VA (Fig. 7) respectively, would explain the over and under prediction in DM yield at both locations. In contrast, good agreement was found between observed and estimated LL and DUL in two soil series at northern sites in IN and IL (Table 8; Fig. 7). This observation suggests a new line of research that should be addressed to clarify to what extent the under or over estimation of these soil water parameters affects the outcome of predicted DM yield in APSIM.

Previous modelling efforts for predicting DM yield of switchgrass were reported. While Grassini *et al.* (2009) demonstrated similar trends in the DM yield predictions (CCC = 0.77), these results were obtained based on a limited number of observations (8) from two northern US environments (Ames, IA and Mead, NE). Additionally, the accuracy of the ALMANAC model (Kiniry *et al.*, 2005) and APSIM to predict DM yield were similar differing by <7%. However, yield values reported by these authors was nearly double what we observed in our study (ca. 17000 vs. 8000 kg DM ha^{-1}) despite comparable dryland conditions. While ALMANAC accounted for 47% of the variability in observed DM yields (Kiniry *et al.*, 2005), when the CCC was calculated from the published results, both models (APSIM and ALMANAC) were poor predictors of DM yield (CCC<0.50) at southern locations (with the exception of Stephenville TX). These authors also observed high year-to-year variability in measured yields at southern locations in the US (TX, LA and AR) and reported that this was not closely associated with variation in rainfall. The lack of fit for the southern locations was evaluated here using our complete dataset. The results showed that the southern locations showed poor fits for observed DM yield as a function of accumulated annual rainfall (Fig. 8a), in contrast with northern locations (Fig. 8b). An additional explanation for the low fit between observed and modelled DM yield at these locations is that the observed DM yields used to validate the model in TX, AR, and LA were derived from the mean of nine cultivars (Cassida *et al.*, 2005; Table S3) in each location. The absence of genotypic parameters for

Table 7 Summary statistics indicating the performance of the Agricultural Production Systems Simulator (APSIM) model in predicting the dry matter yield (kg ha^{-1}) of switchgrass. The data were divided in model calibration and validation subsets. The used data for validation were further split in groups by location (northern and southern) and ecotype (lowland and upland). Northern locations: IN, Indiana; IL, Illinois; TN, Tennessee; NE, Nebraska; IA, Iowa; SD, South Dakota; NY, New York; ND, North Dakota. Southern locations: TX, Texas; VA, Virginia; OK, Oklahoma; LA, Louisiana; AR, Arkansas. The CCC, SB and MSV are the concordance correlation coefficient, bias of the simulation from the measurement and mean square variation, respectively

	Calibration	Validation																
		North								South								
	IN	IL	TN	NE	IA	SD	NY	IN	ND	TX	VA	OK	LA	AR	South	North	Upland*	Lowland*
Observations #	41	16	14	12	19	23	12	12	7	15	12	12	5	3	47	115	101	14
Mean (Observed)	8029	7913	10518	5392	6317	5329	8938	10668	5586	7958	6310	6874	6724	8988	7195	7439	7013	10518
Mean (Modelled)	8055	7400	10786	4960	6360	5371	9999	10570	5988	6654	1391	9357	9015	9879	6458	7496	7040	10786
SD (Observed)	4408	3177	1525	2331	1708	2059	1059	1565	1078	2991	2122	2655	3736	1145	2722	2845	2722	1525
SD (Modelled)	4076	2684	1755	2535	1503	2392	1614	1745	1126	4206	316	2961	2391	524	4288	2987	2836	1755
Testing parameters																		
CCC	0.93	0.93	0.86	0.83	0.73	0.63	0.63	0.50	0.44	−0.07	0.20	−0.55	0.08	0.68	0.01	0.95	0.96	0.64
SB (%)	0	20	9	9	0	0	47	0	12	6	88	22	27	70	2	0	0	9
MSV (%)	100	80	91	91	100	100	53	100	88	94	12	78	73	30	98	100	100	91

*For this dataset the statistical analysis was calculated using only the Northern locations.

Table 8 Summary statistics indicating the performance of HYDRAULIC PROPERTIES CALCULATOR Software (Saxton & Rawls, 2006) in predicting the soil water parameters of ten soil series from different states. Southern locations: Virginia (VA), Texas (TX), Kentucky (KY), Arkansas (AR), Oklahoma (OK) and Louisiana (LA). Northern locations: New Jersey (NJ), Illinois (IL), Indiana (IN) and New York (NY)

	Southern locations						Northern locations			
State	VA	TX	KY	AR	OK	LA	NJ	IL	IN	NY
Series	Cecil	Windthorst	Maury	Bowie	Parsons	Dexter	Holmdel	Flanagan	Chalmers	Collamer
Observations #	16	16	16	18	20	22	20	16	14	14
Testing parameters										
CCC	0.75	0.77	0.80	0.87	0.91	0.92	0.92	0.96	0.97	0.98
SB (%)	37	0	30	0	3	19	13	7	0	14
MSV (%)	63	100	70	100	97	81	87	93	100	86

each cultivar of switchgrass used by these authors, did not allow us to re-parameterize/calibrate/validate the model at the cultivar level. Although the model predicted DM yield of upland switchgrass cultivars better than that of lowland cultivars, the limited number of observations and locations evaluated for lowland ecotypes in this study did not allow us to demonstrate differences in APSIM accuracy by ecotype.

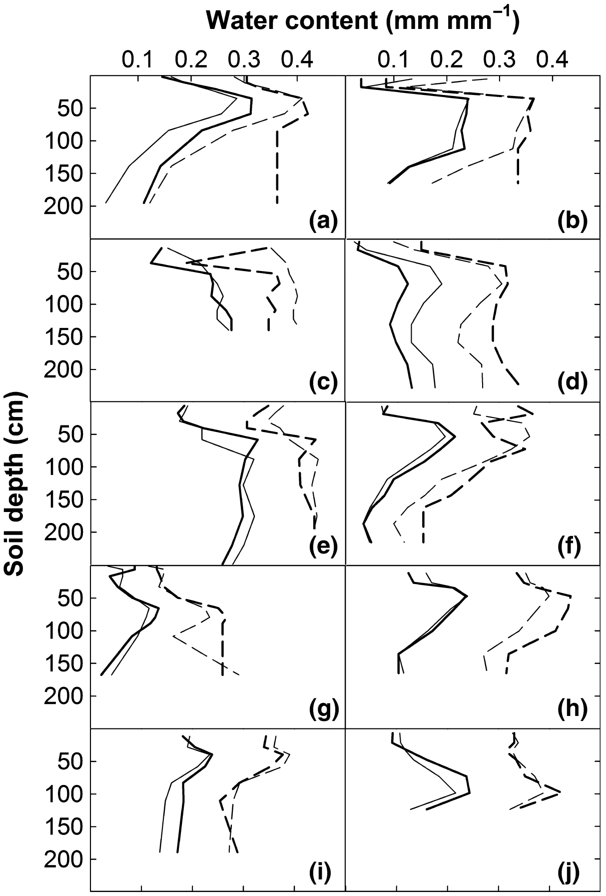

Fig. 7 Drained lower limit (LL, solid lines) and drained upper limit (DUL, dotted lines) observed (thick lines) and estimated (hair lines) by the HYDRAULIC PROPERTIES CALCULATOR Software (Saxton & Rawls, 2006) for the soil series (a) Cecil in VA, (b) Windthorst in TX, (c) Maury in KY, (d) Bowie in AR, (e) Parsons in OK, (f) Dexter in LA, (g) Holmdel in NJ, (h) Flanagan in IL, (i) Chalmers in IN and (j) Collamer in NY.

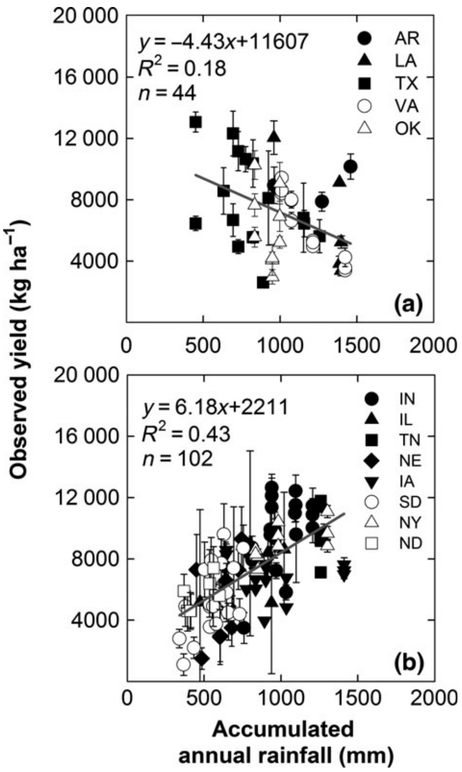

Fig. 8 Relationship between observed dry matter yield of switchgrass vs. accumulated annual rainfall for (a) southern locations and (b) northern locations in US. Northern locations: IN, Indiana; IL, Illinois; TN, Tennessee; NE, Nebraska; IA, Iowa; SD, South Dakota; NY, New York; ND, North Dakota. Southern locations: TX, Texas; VA, Virginia; OK, Oklahoma; LA, Louisiana; AR, Arkansas. Solid grey lines represent linear equation fit to the data. Vertical bars represent the standard deviation in observed values.

Table 9 Summary statistics indicating the cumulative improvement that resulted from re-parameterization of the APSIM *Sugarcane* model for predicting LAI (n = 12) and dry matter yield (n = 20) of *Miscanthus* at Water Quality Field Station, West Lafayette, IN. The parameters modified were *y_rue*, radiation use efficiency and *ratio_root_shoot*, biomass partitioning. The CCC, SB and MSV are the concordance correlation coefficient, bias of the simulation from the measurement and mean square variation, respectively

	Original model	*y_rue*	*ratio_root_shoot*
LAI			
Mean (Observed)	7.6	7.6	7.6
Mean (Modelled)	7.9	7.8	7.3
SD (Observed)	1.2	1.2	1.2
SD (Modelled)	0.2	0.2	0.9
Testing parameters			
CCC	−0.15	−0.03	0.69
SB (%)	5	2	17
MSV (%)	95	98	83
Dry matter yield (kg ha^{-1})			
Mean (Observed)	10 825	10 825	10 825
Mean (Modelled)	9252	11992	9337
SD (Observed)	10 213	10 213	10 213
SD (Modelled)	7970	10 185	7952
Testing parameters			
CCC	0.88	0.90	0.94
SB (%)	12	7	27
MSV (%)	88	93	73

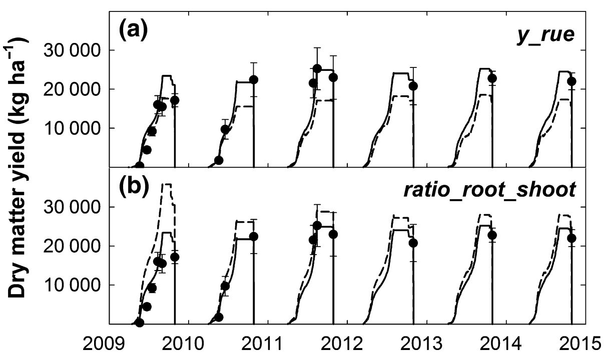

Fig. 9 Modelled pre- (---), post-APSIM *Sugarcane* modification (—) and observed dry matter yield (●) of *Miscanthus* at Water Quality Field Station (West Lafayette, IN). The modified parameters shown in each panel are *y_rue*, radiation use efficiency (a) and *ratio_root_shoot*, ratio root/shoot (b). The effect on dry matter yield was due to the independent modification of each individual parameter. Vertical bars represent the standard deviation in observed values.

Miscanthus

Accurate prediction of *Miscanthus* DM yield using the APSIM *Sugarcane* module required fewer model re-parameterizations when compared to changes made in the

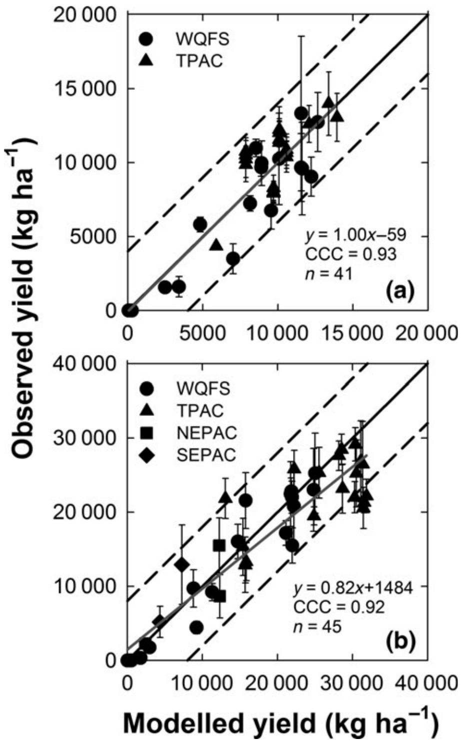

Fig. 10 Scatter plot showing observed vs. modelled dry matter yield for the Indiana sites with calibration data resulting from the re-parameterization of the APSIM model for (a) switchgrass and (b) *Miscanthus*. WQFS, Water Quality Field Station; TPAC, Throckmorton Purdue Agricultural Center; NEPAC, Northeast Purdue Agricultural Center and SEPAC, Southeast Purdue Agricultural Center. Solid black line, dotted line and solid grey line represent 1 : 1 fit (i.e. $y = x$), ± 20% of curve 1 : 1 value and linear equation fit to the data, respectively. Vertical bars represent the standard deviation in observed values where such data were available. The CCC is the concordance correlation coefficient.

APSIM *Lucerne* module parameters to predict DM yield of switchgrass. Sugarcane (*Saccharum officinarum*) shares phenological and physiological attributes with *Miscanthus* due to their close polyphyletic relationship at the subtribe level (Hodkinson *et al*., 2002), so it is not surprising that this APSIM module predicted the DM yield of *Miscanthus*. As with switchgrass, the main plant parameter modified was the RUE. Model DM yield prediction improved when *y_rue* was increased (Fig. 9a). Unlike switchgrass, no change occurred in *Miscanthus* DM yield prediction from changes in *y_extinct_coef* in the three soils evaluated (Fig. 3d). Similarly, DM yield was not sensitive to change in *y_extinct_coef* using SWAT in IN (Trybula *et al*., 2014). In addition, Davey *et al*. (2016) demonstrated that the time period in which increases in the *y_extinct_coef* value had a greatest impact on light interception, and consequently on DM yield, is at the beginning of the growing season before

Table 10 Summary statistics indicating the performance of the Agricultural Production Systems Simulator (APSIM) model in predicting the dry matter yield (kg ha^{-1}) of *Miscanthus*. The data was divided in calibration and validation datasets. IN, Indiana; CA, California; NE, Nebraska; IL, Illinois; VA, Virginia; NJ, New Jersey; KY, Kentucky. The CCC, SB and MSV are the concordance correlation coefficient, bias of the simulation from the measurement and mean square variation, respectively

	Calibration	Validation						
	IN	CA	NE	IL	VA	NJ	KY	Total
Observations #	45	8	15	44	12	17	12	108
Mean (Observed)	15 475	20 421	20 352	18 354	14 926	16 087	17 269	17 927
Mean (Modelled)	17 032	20 101	20 518	18 195	13 883	17 536	16 079	17 841
SD (Observed)	9631	8548	4865	4540	3747	3074	3054	4789
SD (Modelled)	10 924	5213	5321	4025	3469	3488	5442	4653
Testing parameters								
CCC	0.92	0.85	0.69	0.58	0.57	0.46	0.38	0.65
SB (%)	13	1	0	0	10	16	6	0
MSV (%)	87	99	100	100	90	84	94	100

LAI≥4. Therefore, after this stage, further increases in *y_extinct_coef* have little effect on DM yield. Thus, the low sensitivity to this parameter in our study may be based on the constant values of *y_extinct_coef* used for all crop stages.

In a recent study (Zhao *et al.*, 2014) the modelled root biomass of wheat (*Triticum aestivum* L.) was improved trough re-parameterization of the *ratio_root_shoot* parameter using APSIM in China. Likewise, biomass partitioning between roots, rhizomes and shoots for *Miscanthus* has been parameterized for the WIMOVAC model using data from Beale & Long (1997) and this trait has been validated using data from Europe (Miguez, 2007). Based on the mentioned studies, and using data collected by Burks (2013) and Trybula *et al.* (2014) in West Lafayette, IN, the *ratio_root_shoot* parameter was changed in APSIM for all stages, which led to an accurate prediction of DM yield (Fig. 9b; CCC = 0.94).

Similar to switchgrass, sensitivity analysis demonstrated definite trends associated with soil PAWC changes. However, this response differed from switchgrass in that DM yield was greater for the loamy soil than the silty and sandy soils. While the cause is not clear at this time, one plausible explanation is genotypic differences in root exploration between species depending on soil type (Monti & Zatta, 2009). These authors found that *Miscanthus* roots were more concentrated in the top layers of the soil profile as compared with switchgrass, which led to the crop water capture was close and negatively related to root distribution.

Most *Miscanthus* studies for US locations have predicted peak autumn yield (17 500–48 000 kg DM ha^{-1}) and assumed adequate soil moisture and nutrient availability (Heaton *et al.*, 2004; Khanna *et al.*, 2008; Jain *et al.*, 2010; Mishra *et al.*, 2013). However, our predicted DM yields from the validation work for this same region (17 000 kg ha^{-1} at IN to 20 500 kg ha^{-1} at NE) are lower because *Miscanthus* was grown under water and/or nutrient-limiting dryland conditions, (except in CA).

The APSIM *Sugarcane* module was able to satisfactorily predict *Miscanthus* DM yields at IN locations (calibration) and for most locations evaluated (validation) with the exception of NJ and KY. As was discussed for switchgrass, the poor ability of the model to predict DM yield of *Miscanthus* at these two locations was associated with the inaccurate estimation of PAWC. An over-estimation of DUL was found in the Maury soil series at KY (Fig. 7c). In fact, the estimated soil water parameters were not in a satisfactory range as compared with the observed values (0.80 for CCC and 30% for SB) at this site when compared with the soils at IL, IN and NY (0.96–0.98 for CCC and 0–14% for SB). Similarly, a poor fit was found between observed and estimated DUL in the soil layers from 0.5 to 1.5 m in the Holmdel soil series in NJ (Fig. 7g); however, the prediction level of the LL and DUL using the HYDRAULIC PROPERTIES CALCULATOR Software developed by Saxton & Rawls (2006) was acceptable in this soil (0.92 for CCC and 13% for SB).

APSIM model: a promising tool to simulate DM yield for switchgrass and Miscanthus in several US environments

This work was the first attempt to re-parameterize two current APSIM plant modules (*Lucerne* and *Sugarcane*) for predicting the DM yield of switchgrass and *Miscanthus*. Such re-parameterization was conducted based on an extensive literature review and using detailed experimental datasets. We initially focused on the re-parameterization of plant and soil modules and on predicting

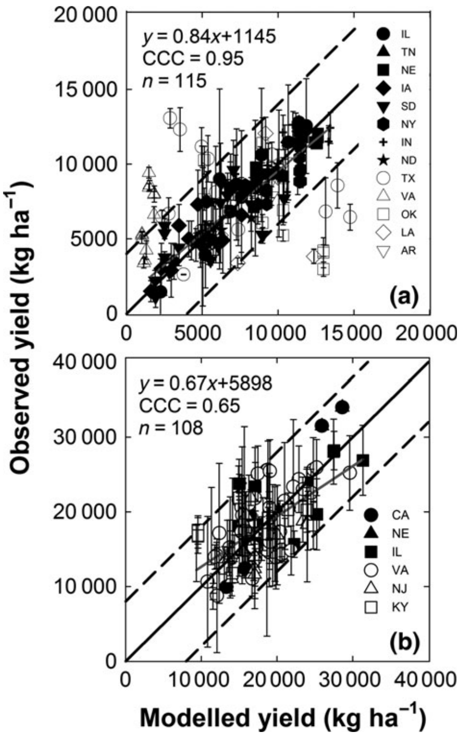

Fig. 11 Scatter plots of observed vs. modelled dry matter yield for all sites with validation data using the re-parameterized APSIM model for (a) switchgrass and (b) *Miscanthus* in different states. ND, North Dakota, NE, Nebraska, IL, Illinois, NY, New York, SD, South Dakota, IA, Iowa, IN, Indiana, TN, Tennessee, AR, Arkansas, TX, Texas, OK, Oklahoma, LA, Louisiana, VA, Virginia, CA, California, KY, Kentucky and NJ, New Jersey. Solid black line, dotted line and solid grey line represent 1 : 1 fit (i.e. $y = x$), ± 20% of curve 1 : 1 value and linear equation fit to the data, respectively. The linear equation, CCC (concordance correlation coefficient) and number of observations (n) correspond to northern locations data and complete dataset for switchgrass and *Miscanthus*, respectively. Vertical bars represent the standard deviation in observed values.

the direction and the magnitude of the DM yield responses.

The study demonstrates:

- The simulation of switchgrass DM yield in northern locations of the US using the re-parameterized APSIM *Lucerne* module had greater accuracy than in southern ones. The improved predictions were associated with a strong, positive association between DM yield and accumulated annual rainfall.
- The original version of the APSIM *Sugarcane* module can be used to accurately simulate the growth and yield of *Miscanthus* in a broad range of geographies and ecosystems within the US that differ in local weather, soil characteristics, and crop management.
- The predictions of the DM yield for *Miscanthus* improved substantially when the physiological parameters (*rue* and *ratio_root_shoot*) of the model were modified.
- PAWC parameterization in a soil profile was critical for explaining DM yield differences for both crops.

This study represents an advance with respect to previous ones to simulate switchgrass and *Miscanthus* because: (i) the DM yield predictions were carried out with the same model (ii) the re-parameterization was started from two existing APSIM plant modules, (iii) the modelled DM yields have been compared against independent datasets, which include contrasting cultivars of switchgrass and environments, and (iv) the average errors associated with the predictions of DM yield at northern locations of switchgrass and *Miscanthus* were extremely low for both the calibration and the validation (26–57 kg ha^{-1} and 1557–86 kg ha^{-1}, respectively). To improve the APSIM accuracy under these environments additional agronomic studies are needed, since only a limited number of locations were utilized for each species. In addition, as our study was based on APSIM calibrations at IN locations, further calibrations of the model using data obtained from other environments is recommended. Nevertheless, these re-parameterized APSIM modules hold promise as tools for predicting switchgrass and *Miscanthus* yields in several US environments.

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Supporting Information

Additional Supporting Information may be found online in the supporting information tab for this article:

Table S1. Summary of climate datasets used for evaluate the NASA-POWER data.
Table S2. Means, standard deviation and variation (VAR) of soil water parameters by texture class used by sensitivity analysis of plant available water capacity (PAWC).
Table S3. Summary of switchgrass datasets used for the calibration/validation of APSIM.
Table S4. Summary of *Miscanthus* datasets used for the calibration/validation of APSIM.
Table S5. Description of actual and estimated soil parameters by location used for the calibration/validation of APSIM.
Table S6. Crop genotype parameterization for the calibration/validation of APSIM.
Table S7. *Ratio_root_shoot* by phenological stage of *Miscanthus* with the range of values calculated based on the aerial and root biomass obtained from two field experiments at Water Quality Field Station at Purdue University (Burks, 2013; Trybula *et al*., 2014). The average *ratio_root_shoot* value by stage was used to re-parameterize the *Sugarcane* APSIM module.